Phenomenological inelastic scattering model for electron transport in mesoscopic devices

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We present a phenomenological inelastic scattering model that allows accurate quantum transport current calculations in semiconductor devices and is applicable to mesoscopic systems such as modern state-of-the-art transistors and beyond-CMOS devices. The model has no fitting parameters and is applicable to systems without significant self-heating effects. It is validated on silicon mobility and resistivity data in the wide range of temperatures (4K-500K), doping densities (10^{18}cm^{-3}-10^{21}cm^{-3}) and sheet doping densities (10^{10}-10^{15}cm^{-2}). When applied to IBM's Lgate=12nm, TSi=5nm GAAFET devices [1], it agrees well with the experimental I-V measurements.

Mesoscopic devices are not made of a single molecule, but still consist of many thousands or even millions of atoms. Just 1nm3 of Si contains about 120 of atoms and the simulation volume of the state-of-the-art GAAFET transistor is about $(50\text{nm})^3$ or about 15 million atoms. Quantum transport simulation of such devices is challenging, but recent progress demonstrates [2-5] that numerically efficient first principles simulations with no fitting parameters can correctly predict the conductive properties of highly-conductive highly-confined Si:P/B systems at cryogenic temperatures, where elastic electrostatic scattering is very strong, but inelastic scattering effects can be ignored. In this work we introduce a model that allows sufficiently accurate and very simple description of inelastic scattering effects on the current in such mesoscopic systems, thus extending the range of efficient predictive quantum transport simulations to elevated and room temperatures. The idea is to approximate the current spectrum affected by the two-body inelastic scattering collisions by weighting the ballistic current spectrum with the ballisticity factor $B(E)$, $i_{eff}(E)=i_{ballistic}(E)\cdot B(E)$. The ballisticity factor is assumed to be proportional to the number of phonons with the comparable to electron energies. Effectively, the model dampens the computed ballistic current spectrum for those frequencies where phonon population is high, leaving the rest of the current spectrum unmodified. Remarkably, this exceptionally simple scheme for accounting of inelastic scattering provides an excellent match to the experiment, as can be seen from Figure 1, without using any fitting parameters. We show that the model also allows to recover the electron mobility values in silicon thin films for a wide range of temperatures and doping values as illustrated in Figure 3.

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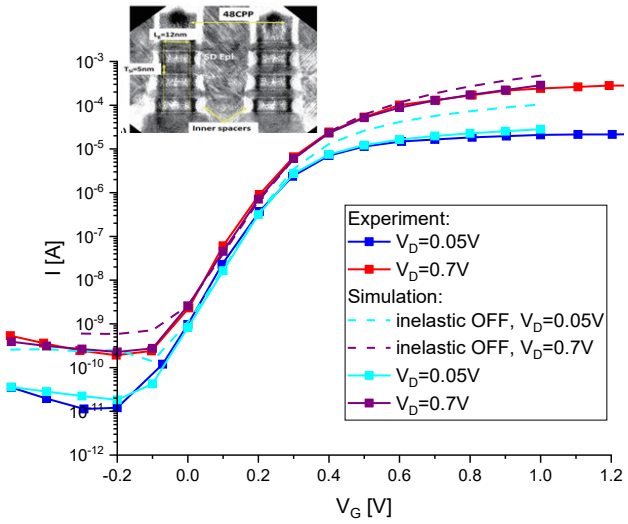

Fig. 1. Electrical characteristics of IBM's GAAFET [1] device: experimental measurements vs first principles simulation results. Dashed lines: no inelastic scattering (ballistic), solid lines: using the inelastic scattering model. Note that the current spectrum is effectively reduced for those energies, where phonon population is high, as a function of the gate voltage and the corresponding effective potential barrier, shown in Figure 2.

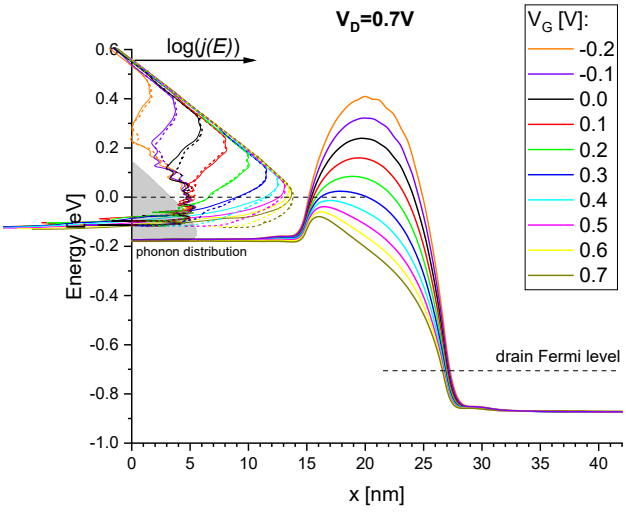

Fig. 2. Effective 1D potential (conduction band edge) from the source (left side) to the channel (middle) and the drain (right side) is shown for different gate voltages (solid color curves); V_D=0.7V. The current density spectrum j(E) is shown in semi-log scale for each gate voltage (solid color curves); the ballistic current spectrum case is also shown using the dashed lines; the grey area represents the phonon distribution $pDOS(E) \cdot f_{B-E}(E)$ expressed as a function of the electron energy.

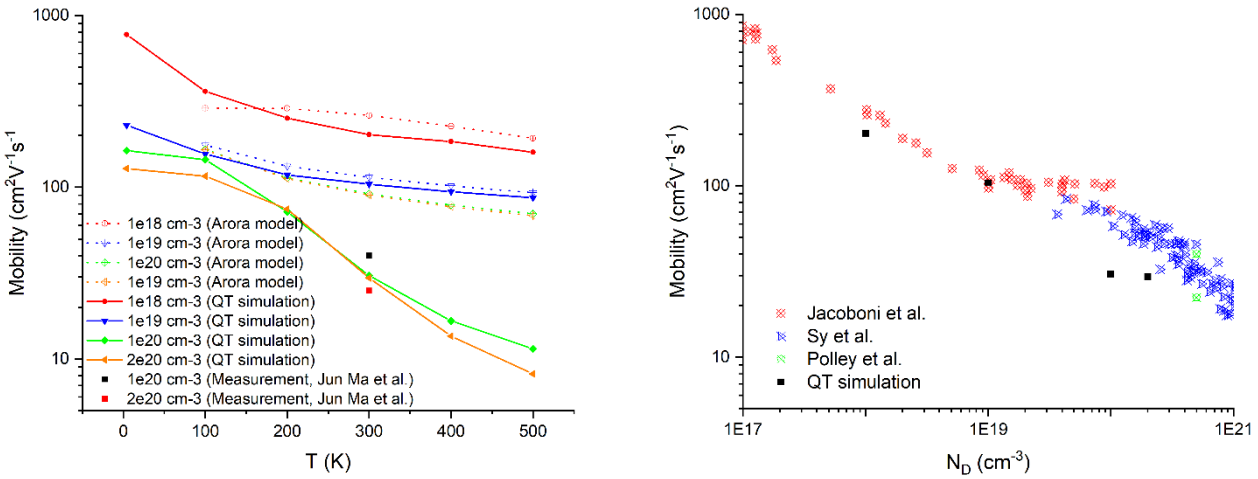

Fig. 3. Left panel: Comparison of the predicted electron mobilities vs temperature between our quantum transport simulations and the Arora model and experimental data for different doping densities; Right panel: Comparison of the electron mobilities predicted by our framework with experimental data at room temperature (300K). Note that here the computed mobility is extracted assuming a very thin (~5nm) silicon film, which lowers the mobility value compared to the bulk values for high temperatures and doping concentrations.